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13. ABSTRACT *(Maximum 200 words)*

The purpose of the proposed research is to develop new numerical methods for computing propagating phase boundaries in solids undergoiong phase transformations, such as the austenite-martensite phase transitions. We are especially interested in understanding how small scale structures, such as tip splitting and cusp formation, are dynamically generated in the process of energy minimization.

Another objective of this project is to develop innovative numerical schemes for computing multiscale solutions on a coarse finite element grid. The purpose of this study is to study scattering and wave propagation in strongly heterogeneous media.

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Annual Report for AFOSR grant F49620-94-1-0215

Thomas Y. Hou
Applied Math, Caltech

The focus of our research has shifted to develop innovative numerical schemes for computing multiscale solutions on a coarse finite element grid. The purpose of this study is to study scattering and wave propagation in strongly heterogeneous media.

Many problems of fundamental and practical importance have multiple scale solutions. Such solutions are typically found in composite materials, transport in porous media, wave propagation in random media, and wave scattering in ocean. In order to obtain accurate numerical solutions using a traditional finite element method, one has to resolve the small scales in the physical solution. This is often impossible for practical computations. Here we consider an alternative approach based on finite element approximations. Our finite element method is different from the conventional finite element method in the sense that the local microstructures of the differential operators are incorporated in the finite element base functions. Through the coupling of the global stiffness matrix, the small scale information in the base functions interacts with the large scale.

In our method, the base functions are constructed from the leading order homogeneous diffusion operator in each element. As a consequence, the base functions are adapted to the local properties of the differential operator. In the case of two-scale periodic structures, we have proved that the multiscale method indeed converges to the correct solution independent of the small scale in the homogenization limit.

One important property of these oscillatory base functions is that they are independent from each other and can be constructed independently. In effect, we break a large scale computation into many smaller and independent pieces, which can be carried out in perfectly parallel. Thus, the size of the computation is drastically reduced. Another advantage of our approach is that it can handle general multiscale problems without the requirement of scale separation. Such assumption is often required in the theory of homogenization.

A common difficulty in numerical upscaling methods is that large errors result from the "resonance" between the grid scale and the scales of the continuous problem. This is revealed by our analysis. For the two-scale problem, the error due to the resonance manifests as a ratio between the wavelength of the small scale oscillation and the grid size; the error becomes large when the two scales are close. A deeper analysis shows that the boundary layer in the first order corrector seems to be the main source of the resonance effect. By a judicious choice of boundary conditions for the base function, we can eliminate the boundary layer in the first order corrector. This would give a nice conservative difference structure in the discretization, which in turn leads to *cancellation of resonance errors* and gives an improved rate of convergence independent of the small scales in the solution.

Motivated by our analysis mentioned above, here we propose an *over-sampling* method to overcome the difficulty due to scale resonance. The idea is quite simple and easy to implement. Since the boundary layer in the first order corrector is thin, $O(\epsilon)$, we can sample in a domain with size larger than $h + \epsilon$ and use only the interior sampled information to construct the bases; here, h is the mesh size and ϵ is the small scale in the solution. By doing this, the boundary layer in the larger domain has no influence on the base functions. Now the corresponding first order

correctors are free of boundary layers. As a result, we obtain an improved rate of convergence which is independent of the small scale.

We have demonstrated convincingly the accuracy and efficiency of our method through extensive numerical experiments, which include wave propagation in strongly heterogeneous media, steady conduction through fiber composites and flows through random media with normal and fractal porosity distributions, and turbulent transport problems.

Personnel Supported

This grant has supported one-month summer salary for Profs. Thomas Y. Hou from Caltech and Philippe LeFloch from Ecole Polytechnique/France.

Interactions/Transitions:

The work on multiscale finite element methods has been presented by Hou in the Fourth SIAM Meeting on Mathematical and Computational Issues on Geosiences in Alberquerque in June of 97. Our results were very well received. In our subsequent visit to the Earth and Geoscience Division in Los Alamos, the experts there were very enthusiastic about our results and would like to have a long term interaction with us on various applications of our method. Hou also presented this work in the first International Congress of Analysis, Applications and Computations in Delaware. The work was equally well received. The work on phase boundaries has been presented by Prof. LeFloch at the International Conference on Hyperbolic PDE's in Hong Kong in June of 96, and has been presented by Prof. P. Rosakis (our collaborator) at the annual ASME material science meeting in 1995.

New Discoveries, Inventions or Patent Disclosures: None.

Publications

1. T. Y. Hou, P. LeFloch, and P. Rosakis, *Dynamics of Phase Interfaces: A Level Set Approach,* preprint, 1997, submitted to J. Comp. Phys.
2. B. Hayes and P. LeFloch, *Non-Classical Shock Waves in Scalar Conservation Laws,* to appear in Archiove for Rational Mechanics and Analysis, 1996.
3. T. Y. Hou and X. H. Wu, *A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media,* J. Comput. Phys., Vol. 134, pp. 169-189, 1997.

Honors and Awards:

Hou was recently invited to give a 45-Minute Lecture at the International Congress of Mathematicians in Berlin, 1998. This is considered a very high honor for mathematicians. He also received the Feng Kang Prize in Scientific Computing in August of 1997. In addition, he was invited as a visiting professor (one-month) in University of Paris XI and Mittag-Leffler Institute in 1997.

Killer Chart for F49620-94-1-0215

Thomas Y. Hou

Here we would like to demonstrate our recent results obtained using our multiscale finite element method and the level set method. The applications are for wave propagation through a multiscale geometry and propagation of phase boundaries respectively.

One of the important applications of our multiscale finite element method is for wave propagation in a complicated, and singular geometry. This problem is very difficult to deal with by conventional finite element method due to the geometric singularity and the high contrast of scales. The purpose of our method is to capture the effect of small scales on the large scales without resolving the small scales globally. We illustrate our computational results from Figures 1 to 4. The results are quite encouraging.

In Figure 1, we plot the discontinuous wave speed Coefficient, a_ϵ, in the wave equation with discontinuous coefficient, i.e. $u_{tt} = \nabla \cdot a_\epsilon(x) \nabla u$. The dimension of the narrow channel is 0.04×0.1 embedded in a unit square. The minimum wave speed is 0.05. We plot the solution to the wave equation at $t = 0.7$ using a relatively fine resolution, $N = 256 \times 256$, in Figure 2. Linear finite element would have a lot of difficulty to get an accurate solution even at this fine level of grid. We observe that most of waves get reflected by the channel, part of waves leak through the narrow channel. We repeat the same calculation in Figure 3, using the same initial data as in Figure 2, but with a coarser grid, $N = 64 \times 64$. One can see that we still capture the main feature. We repeat the same calculation using an even coarser grid, $N = 32 \times 32$ in Figure 4. There is about one grid point inside the narrow channel. We still capture the main feature.

Next we demonstrate some of our computational results for phase boundaries using the level set method. In Figure 5, we plot the early stage of propagation of phase boundaries started from a small inclusion. A narrow needle like shape is formed quickly during the evolution. In Figure 6, we observe splitting of the phase boundary near the wall. Energy is decreased during this process. And secondary splitting is observed near the wall. In Figure 7, we observe that the splitted phase boundaries travel inward, and eventually experience a topological change. At the exact moment of topological transition, the energy experiences a sudden drop. Total energy as a function of time is plotted in Figure 8. The sudden decrease is due to the topological change in the phase boundary. In Figure 9. we plot another example of propagation of phase boundaries corresponding to a different loading. More fine structures are created near the wall. Energy decreases during this process.

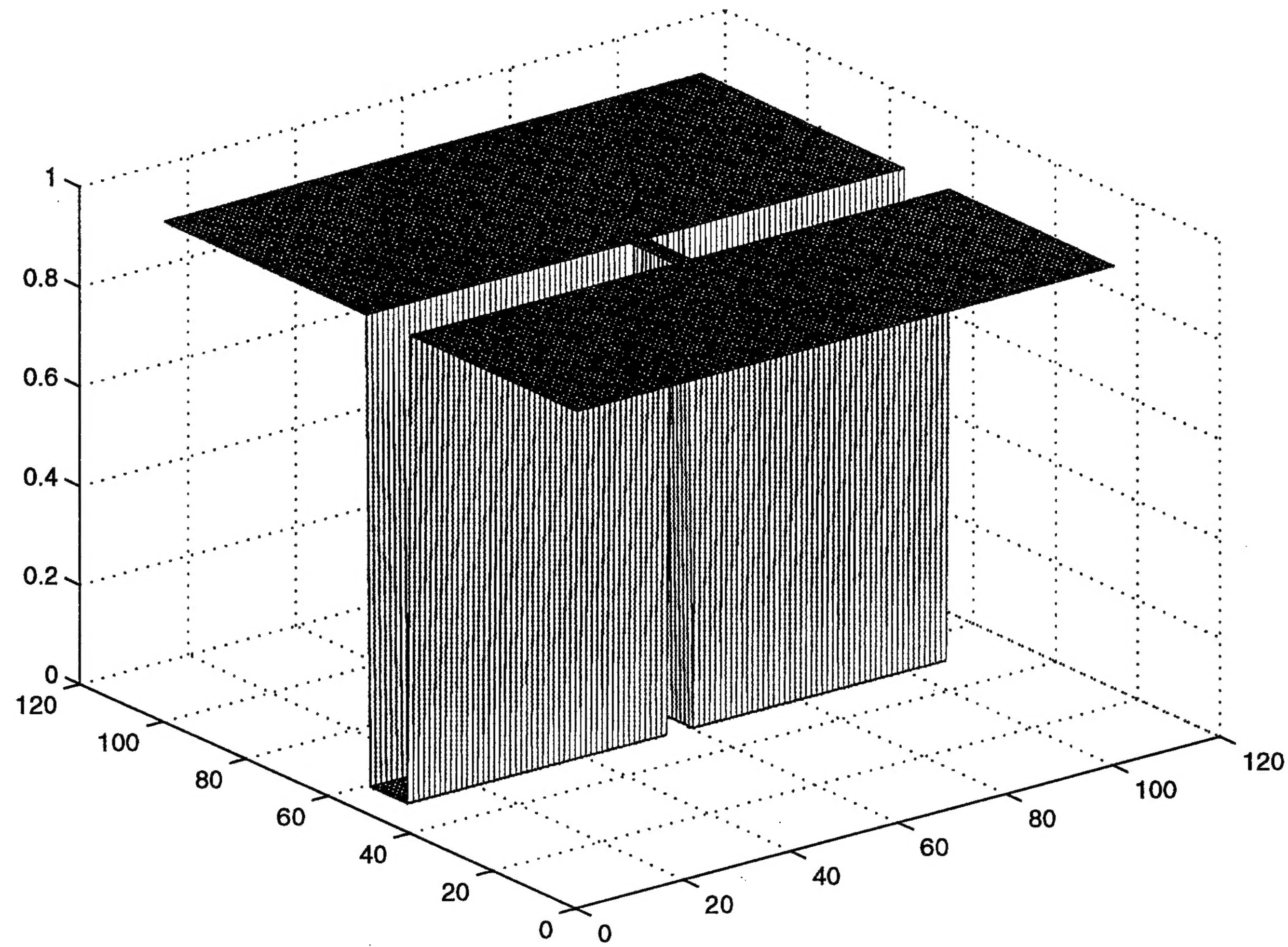

Figure 1. Discontinuous wave speed Coefficient, a_ϵ, in $u_{tt} = \nabla \cdot a_\epsilon(x) \nabla u$.

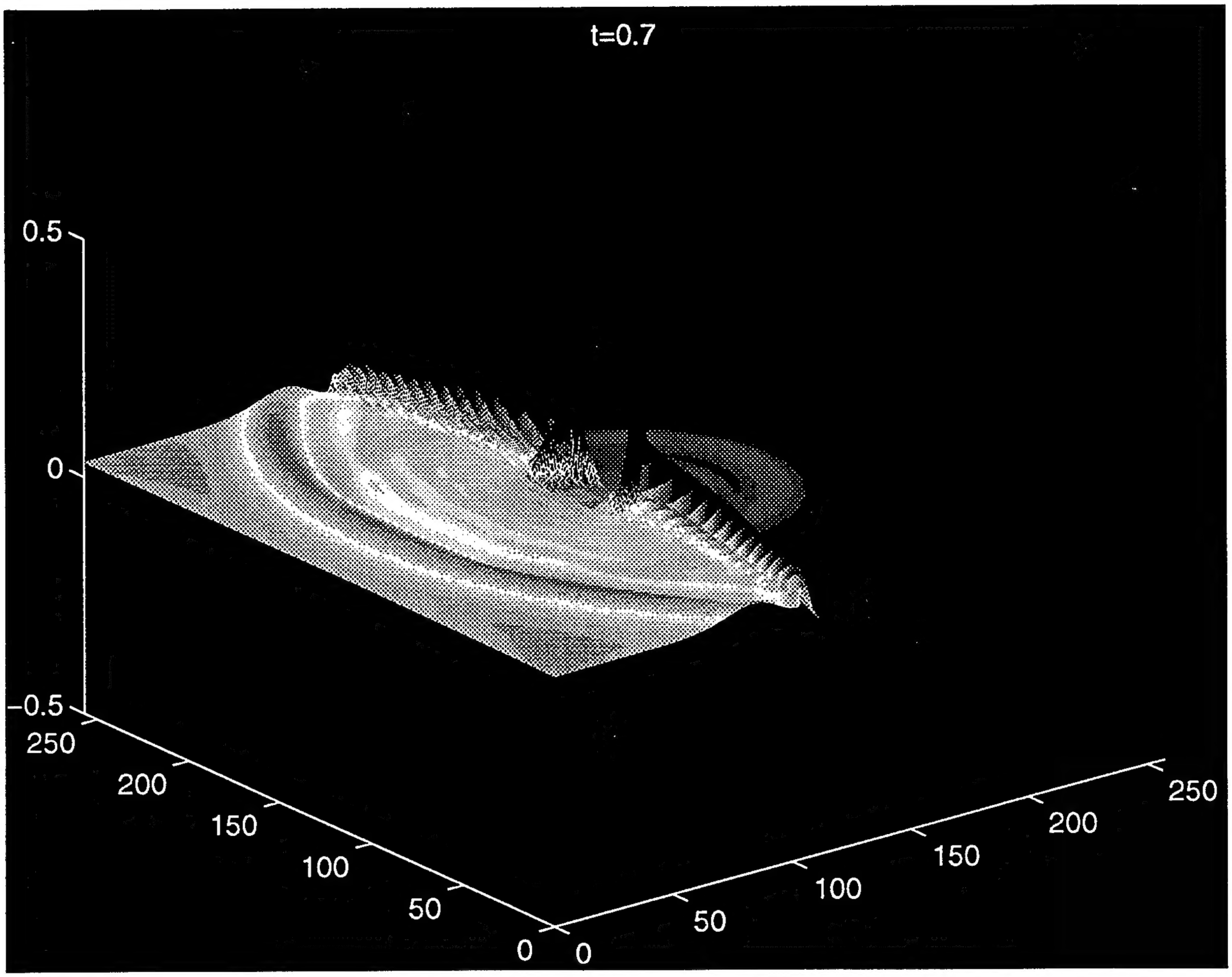

Figure 2. Solution to the wave equation at $t = 0.7$, most of waves get reflected, part of waves leak through the narrow channel. $N = 256 \times 256$.

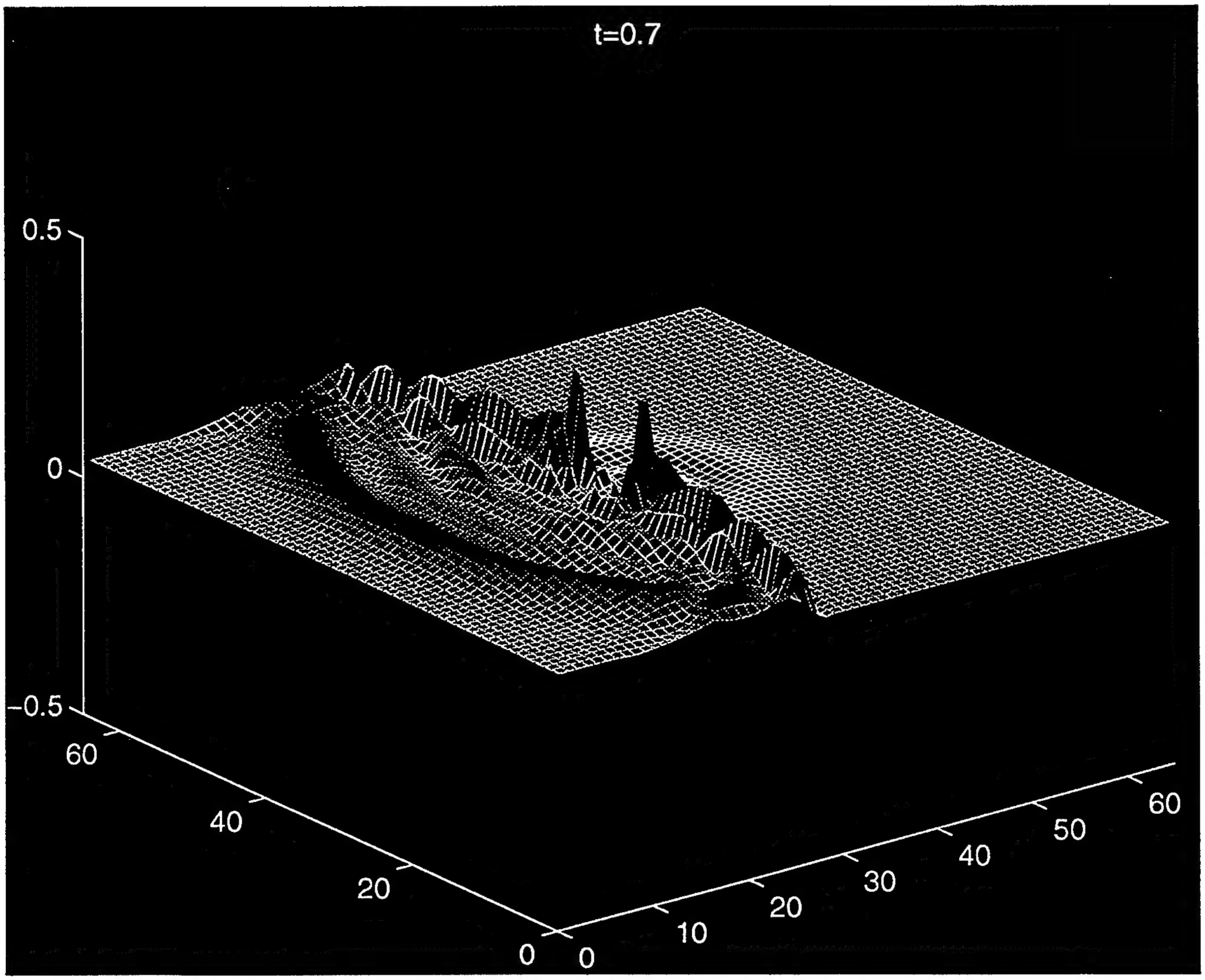

Figure 3. The same calculation as in Figure 2, but with a coarser grid, $N = 64 \times 64$. We still capture the main feature.

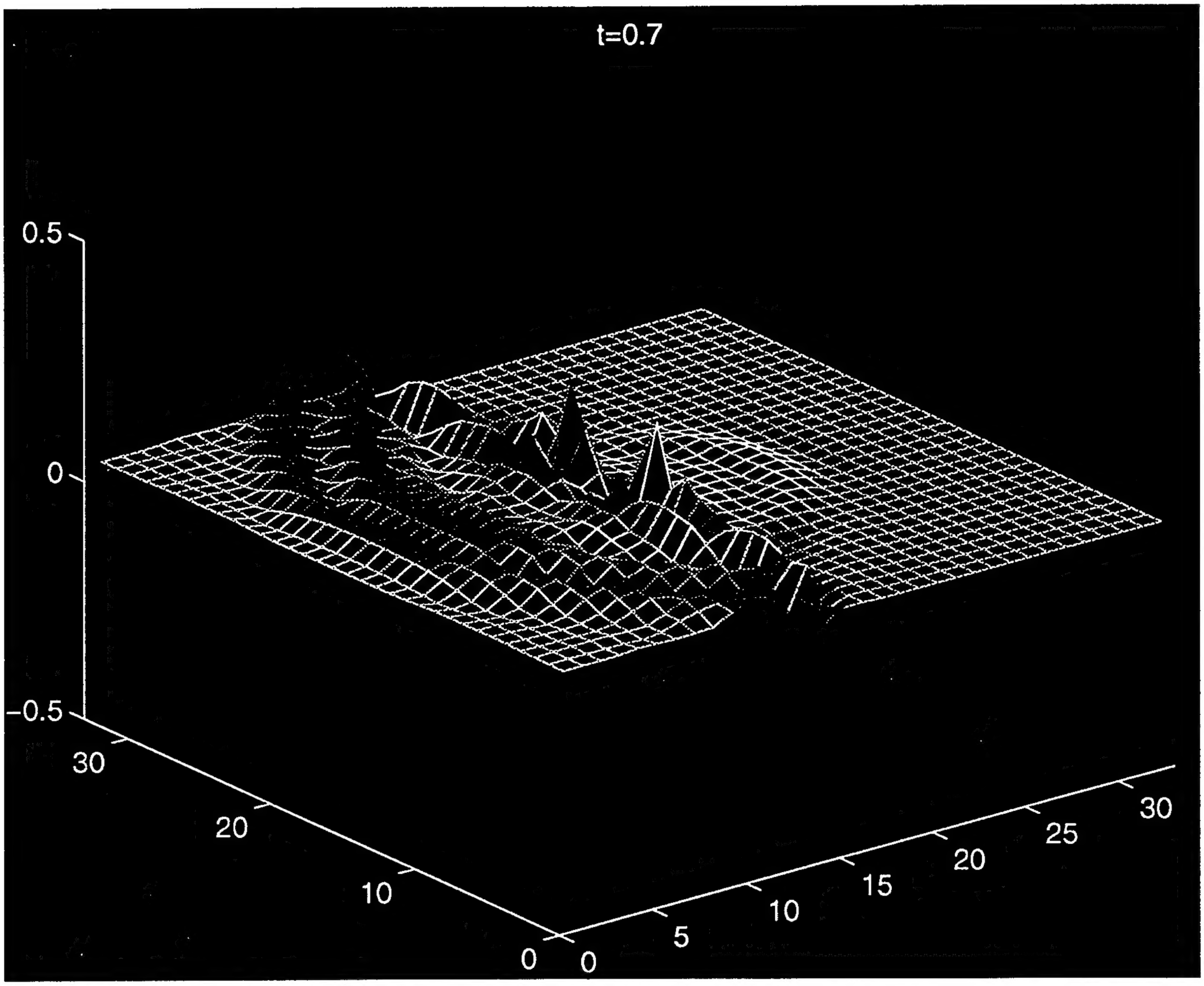

Figure 4. The same calculation as in Figure 2, but with an even coarser grid, $N = 32 \times 32$. There is about one grid point inside the narrow channel. We still capture the main feature.

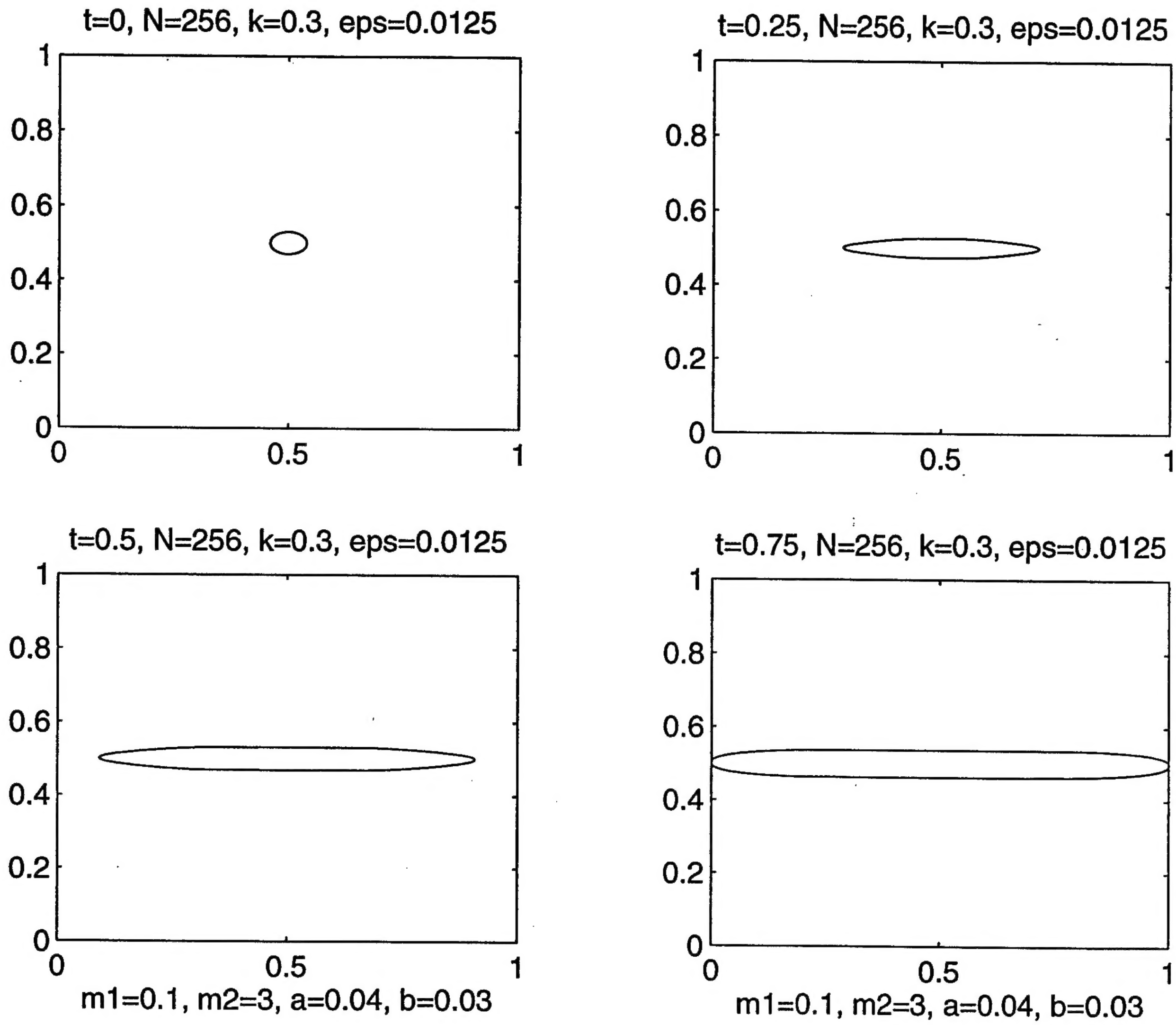

Figure 5. Propagation of phase boundaries started from a small inclusion. A narrow needle like shape is formed quickly during the evolution.

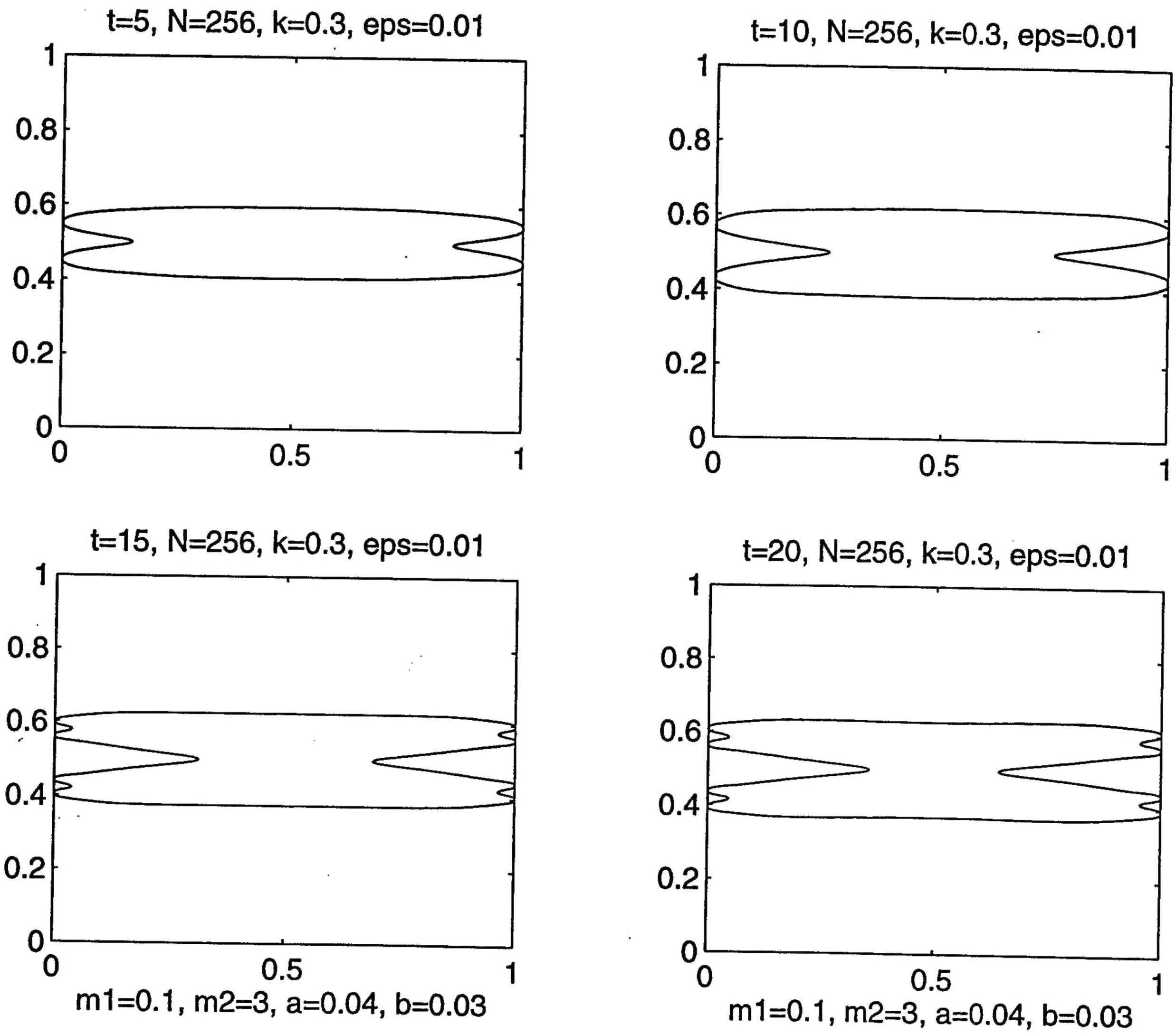

Figure 6. We observe splitting of the phase boundary near the wall. Energy is decreased during this process. And secondary splitting is observed near the wall.

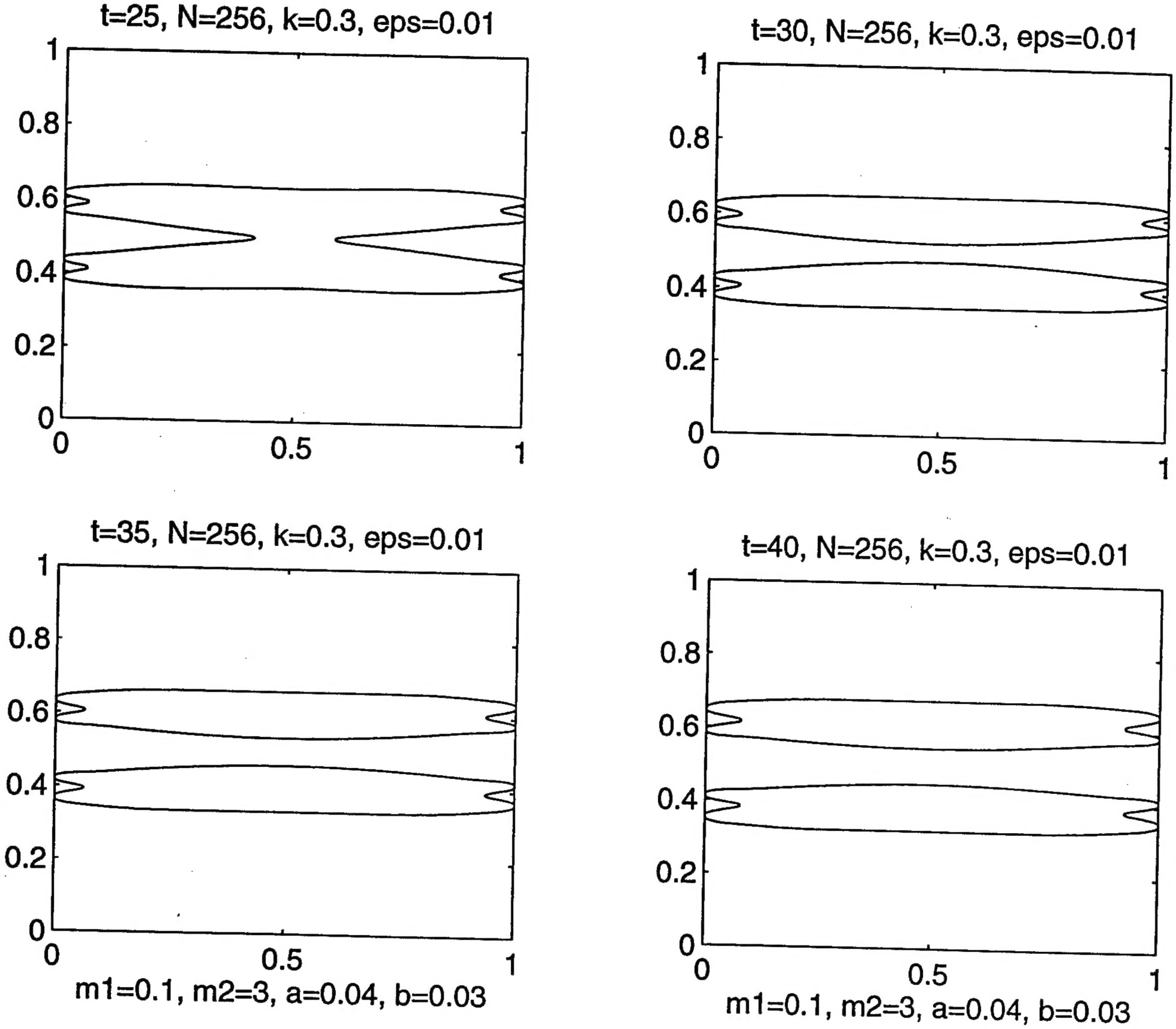

Figure 7. The splitted phase boundaries travel inward, and eventually experience a topological change. At the exact moment of totological transition, the energy experiences a sudden drop. See Figure 8.

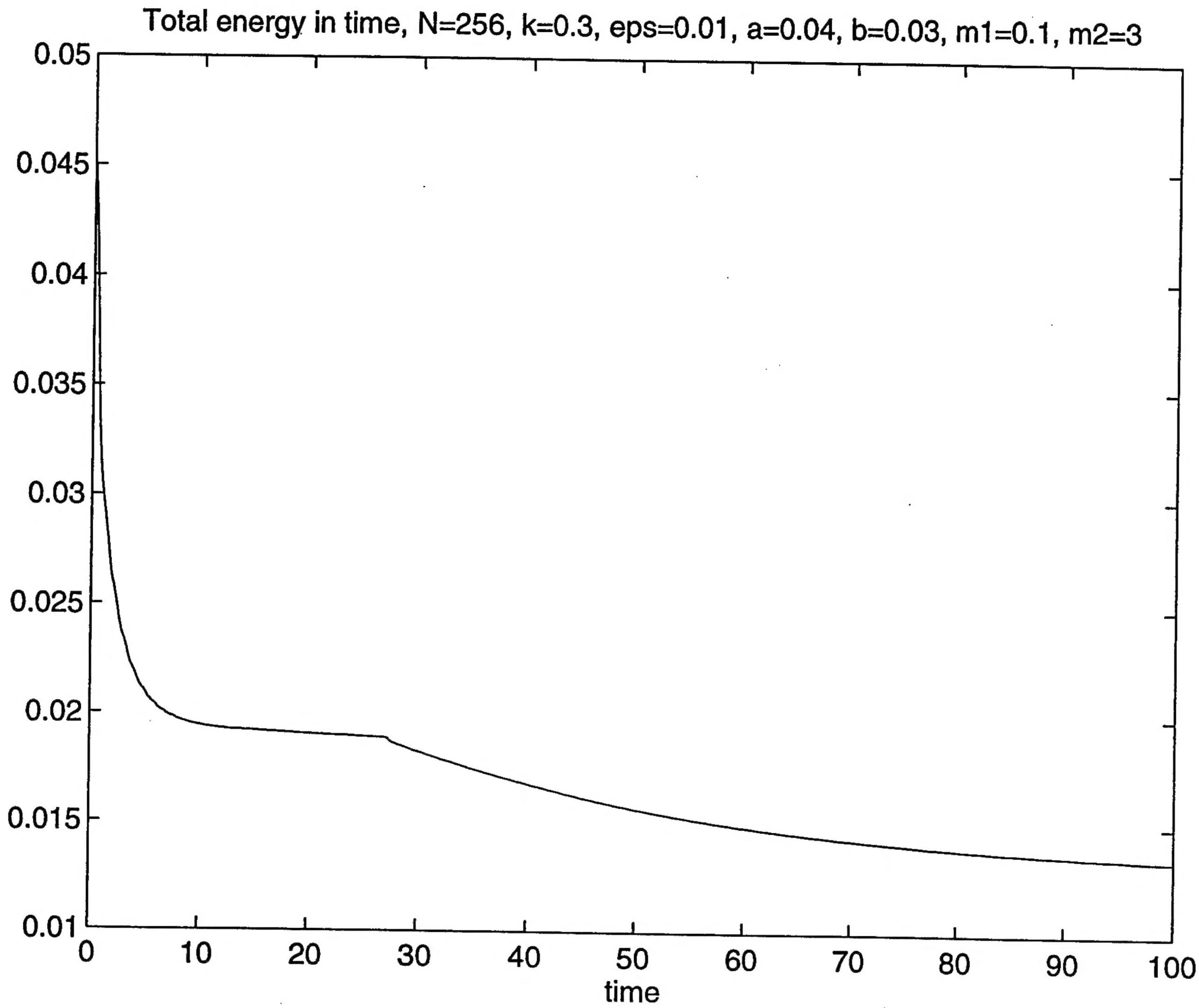

Figure 8. Total energy as a function of time. The sudden decrease is due to the topological change in the phase boundary.

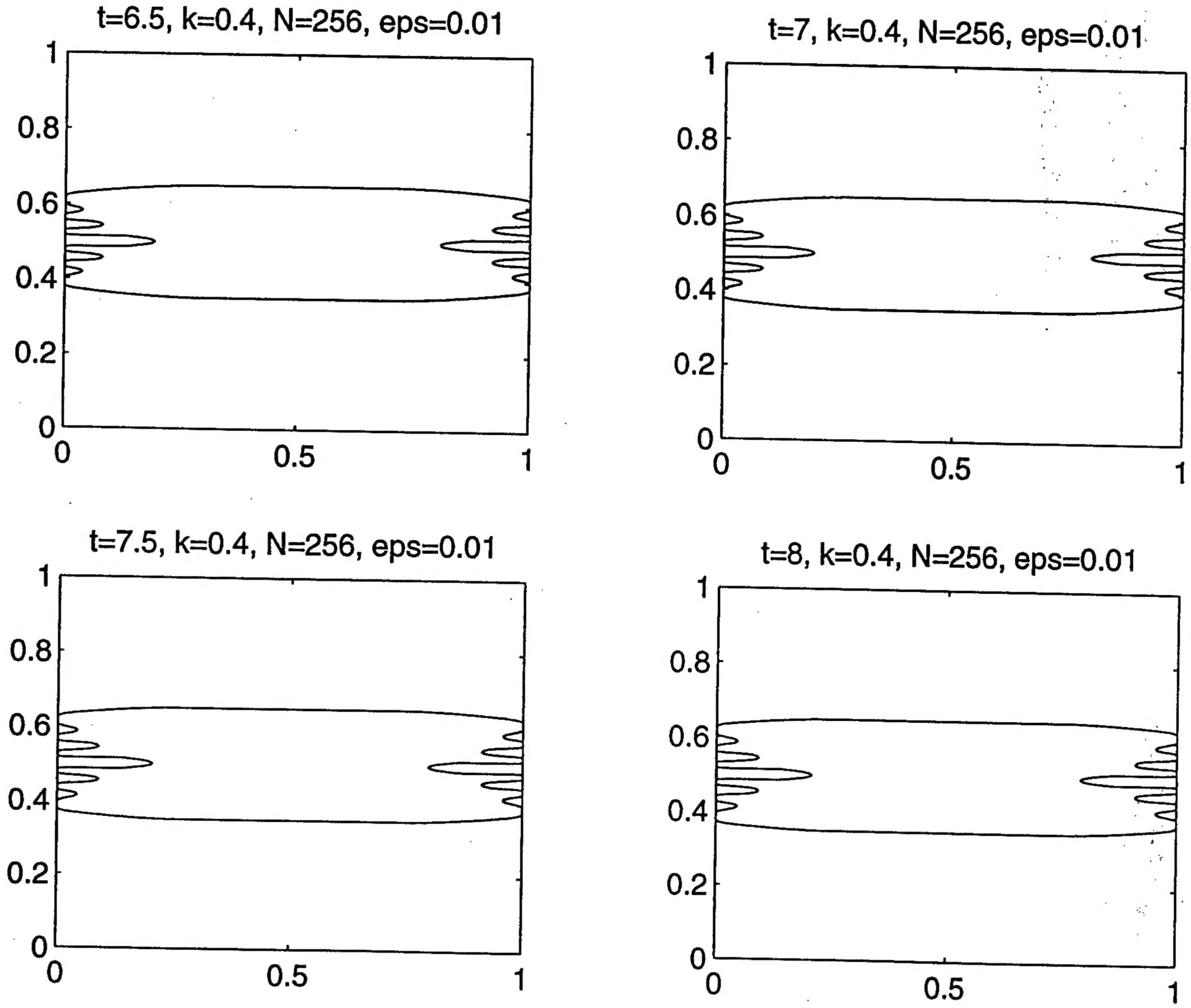

Figure 9. Phase boundary corresponding to a different loading. More fine structures are created near the wall. Energy decreases during this process.